REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	July 1995	Final 1 May 1992 - 30 April 1995

4. TITLE AND SUBTITLE
Quantum Transport in Solids: Two-Electron Processes

5. FUNDING NUMBERS
DAAL03-89-D-0003

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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
ARO 30549.1-EL

11. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy, or decision, unless so designated by other documentation.

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

The central objective of this research program has been to study theoretically the underlying principles of quantum transport in solids. The area of research investigated has emphasized the understanding of two-electron processes in quantum transport. The problems have been treated analytically to the extent possible through the use of dynamical localized Wannier functions. These results have been and are being incorporated in a full quantum transport theory that includes dielectric screening, dynamical high-field effects, and electron-electron interactions. The research under this grant has culminated in the formulation of a theory describing Bloch electron transport in inhomogeneous electric fields due to localized impurities. Based on this model, a variety of novel field-controlled current modulators have been defined; the U.S. Army has filed for a patent based on these concepts.

14. SUBJECT TERMS
Bloch electron dynamics; Wannier functions; Electron transport in inhomogeneous electric fields

15. NUMBER OF PAGES
12

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

QUANTUM TRANSPORT IN SOLIDS: TWO-ELECTRON PROCESSES

FINAL REPORT

GERALD J. IAFRATE

1 JUNE 1995

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DAAL03-89-D-0003

NORTH CAROLINA STATE UNIVERSITY

1A. STATEMENT OF PROBLEM STUDIED

During the past decade, as microelectronics technology has continued to pursue the scaling down of IC device dimensions into the submicron and ultrasubmicron regions, many new and interesting questions have emerged[1] concerning hot-carrier physics, particularly with regard to the solid-state dynamics and quantum transport of carriers in crystalline solids subjected to high electric fields.

In this research, we have studied electric field-assisted transport of charge carriers in solids with specific emphasis on the role of electron-electron interactions in the dynamical processes. Specific interest in this study arises from issues and questions relevant to the simultaneous role of high-electric fields and electron scattering processes in influencing transport, electron relaxation, noise generation, and ionization processes in quantum-wells, tunnel barriers, and superlattices[2].

Prior to this research program we had developed[3] a novel formalism for treating Bloch electron dynamics and quantum transport in inhomogeneous electric fields of arbitrary strength and time dependence. In this formalism, the electric field is described through the use of the vector potential, a gauge choice which leads to a natural temporal description of Bloch electron dynamics in the presence of electric fields. In addition, a basis set of dynamical localized Wannier functions had been established[4] and utilized to derive a quantum "Boltzmann equation" which included band-structure effects and explicit band-mixing transients such as effective mass dressing and Zener tunneling; the application of this formalism to quantum transport in spatially localized inhomogeneous electric fields such as occur in problems involving tunneling through "band-engineered" tunneling barriers and impurity scattering had been presented[5].

In this work, we have extended this previously established methodology to treat a variety of physical systems including multiband systems with uniform electric fields and systems containing localized impurities.

1B. SUMMARY OF MOST IMPORTANT RESULTS

During this initial period of research, a novel multi-band theory of Bloch electron dynamics in homogeneous electric fields of arbitrary strength and time-dependence was formulated. In the formalism, the electric field is described through the use of the vector potential. Multi-band coupling is treated through the use of the Wigner-Weisskopf approximation, thus allowing for a Bloch electron transition out of the initial band due to the power absorbed by the electric field; also, the approximation ensures conservation of total transition probability over the complete set of excited bands. The choice of the vector potential gauge leads to a natural set of extended time-dependent basis functions for describing Bloch electron dynamics in a homogeneous electric field; an associated basis set of localized, electric field-dependent Wannier and related envelope functions are developed and utilized in the analysis to demonstrate the inherent localization manifest in Bloch dynamics in the presence of strong electric fields. From the theory, a generalized Zener tunneling time is derived in terms of the applied uniform electric field and the relevant band parameters; specific results are derived using a nearest-neighbor tight-binding, multi-band model, and are shown to have an equivalent parametric dependence on electric field to that of the well-known Kane's two-band model. Further, the analysis shows an electric field-enhanced broadening of the excited state probability amplitudes, thus resulting in lattice space delocalization and the smearing of discrete, Stark-ladder and band-to-band transitions due to the presence of the electric field.

As a result of this grant, research has been completed that resulted in the formulation and publication of a multiband theory of Bloch electron dynamics in a uniform electric field of arbitrary strength. In this formalism, the electric field is described through the use of the vector potential. Multiband coupling is treated through the use of the Wigner-Weisskopf approximation, thus allowing for a Bloch-electron transition out of the initial band due to the power absorbed by the electric field; also, the approximation insures conservation of total transition probability over the complete set of excited bands. The choice of the vector-potential gauge leads to a natural set of extended time-dependent basis functions for describing Bloch-electron dynamics in a homogeneous electric field; an associated basis set of localized, electric-field-dependent Wannier and related envelope functions has been utilized in the analysis to demonstrate the inherent localization manifest in Bloch dynamics in the presence of relatively strong electric fields. From the theory, a generalized Zener tunneling time has been derived in terms of the applied uniform electric field and the relevant band parameters; specific results have been derived from the general theory using a nearest-neighbor tight-binding, multiband model, and were shown to have identical parametric dependence on electric field, but different, more realistic dependence on the appropriate band-structure parameters than those of the well-known Kane and effective-mass two-band model. Further, the analysis shows an electric-field-enhanced broadening of the excited-state probability amplitudes, thus resulting in spatial lattice delocalization and the onset of smearing of discrete, Stark-ladder, and band-to-band transitions due to the presence of the electric field. In

addition, it is predicted that the velocities of a Bloch oscillation will be observed only for the electron that is initially in a Bloch state before Zener tunneling. Further, the influence of electric fields on resonant tunneling structures has been examined.

During this research effort we have also formulated a theory for describing Bloch electron transport in inhomogeneous electric fields due to localized impurities. Furthermore, this theory has been used to model the dynamics of a Bloch electron in homogeneous electric fields in the presence of such impurities. Based on this model, we have predicted that field-controlled current modulators can be realized on the basis of the barrier-strength tuning that occurs when the Bloch frequency is an integral multiple of the frequency of the applied field; this phenomenon has been used to define a wide variety of novel field-controlled current modulators as documented in our invention disclosure filed with Docket Number CECOM-5153 in 1994.

1C. LIST OF ALL PUBLICATIONS AND TECHNICAL REPORTS

Jun He and Gerald J. Iafrate, "Effects on Band-structure and Electric Fields on Resonant Tunneling Dynamics," NATO Advanced Study Institute (July 1994), to appear in Quantum Transport in Ultrasmall Devices, Kluwer Publishing, Inc.

Jun He and Gerald J. Iafrate, "Multiband Theory of Bloch-Electron Dynamics in a Homogeneous Electric Field," Physical Review B, 50, 7553 (1994).

Jun He and Gerald J. Iafrate, "Bloch Electron Dynamics in a Superimposed Uniform and Oscillatory Electric Field," Bulletin of the American Physical Society, 39, 894 (1994); to be published.

Jun He, Gerald J. Iafrate and M.A. Littlejohn, "Multiband Theory of Bloch Electron Dynamics in Electric Fields," Semiconductor Science and Technology, 9, 815 (1994).

V. Sankaran, K.W. Kim and G.J. Iafrate, "Tight-binding Calculation of Linear Optical Properties of $In_{0.53}Ga_{0.47}As$ Alloys and Heterostructures," Chapter 7 of Institute of Physics Conference Series, No. 141, IOP Publishing Ltd. (1995).

G.J. Iafrate and Jun He, "Effects of Electric Fields on Resonant Tunneling," Bull. Am. Phys. Soc., 39, R21 8, 894 (1994); to be published in more complete form.

Jun He and G.J. Iafrate, "Bloch Electron Dynamics in a Superimposed Uniform and Oscillatory Electric Field," Bull. Am. Phys. Soc., 39, R21 9, 894 (1994); to be published in more complete form.

2. REPORT OF INVENTION

Gerald J. Iafrate, Jun He, Mitra Dutta, and Michael A. Stroscio, "Field Controlled Current Modulators Based on Tunable Barrier Strengths," Attorney Docket No.: CECOM-5153, 1994.

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5. "Quantum Transport and Dynamics for Bloch Electrons in Electric Fields", G.J. Iafrate, J.B. Krieger and J. Li, NATO Advanced Study Institute on Electronic Properties of Multilayers and Low Dimensional Semiconductor Structures, Castera-Verduzan, France, Plenum Press, 1989.

4. APPENDIX OF COVER PAGES FOR THREE OF THE KEY PUBLICATIONS UNDER THIS GRANT

Multiband theory of Bloch-electron dynamics in a homogeneous electric field

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(Received 24 May 1993; revised manuscript received 20 April 1994)

A multiband theory of Bloch electron dynamics in a uniform electric field of arbitrary strength is presented. In this formalism, the electric field is described through the use of the vector potential. Multiband coupling is treated through the use of the Wigner-Weisskopf approximation, thus allowing for a Bloch-electron transition out of the initial band due to the power absorbed by the electric field; also, the approximation insures conservation of total transition probability over the complete set of excited bands. The choice of the vector-potential gauge leads to a natural set of extended time-dependent basis functions for describing Bloch-electron dynamics in a homogeneous electric field; an associated basis set of localized, electric-field-dependent Wannier and related envelope functions are utilized in the analysis to demonstrate the inherent localization manifest in Bloch dynamics in the presence of relatively strong electric fields. From the theory, a generalized Zener tunneling time is derived in terms of the applied uniform electric field and the relevant band parameters; specific results are derived from the general theory using a nearest-neighbor tight-binding, multiband model, and are shown to have identical parametric dependence on electric field, but different, more realistic dependence on the appropriate band-structure parameters than those of the well-known Kane and effective-mass two-band model. Further, the analysis shows an electric-field-enhanced broadening of the excited-state probability amplitudes, thus resulting in spatial lattice delocalization and the onset of smearing of discrete, Stark-ladder, and band-to-band transitions due to the presence of the electric field.

I. INTRODUCTION

Bloch-electron dynamics in a homogeneous electric field has been a subject of great interest dating back to the earliest applications of quantum mechanics to solid-state physics.[1-3] Even more recently, as modern fabrication technologies continue to drive the study of solid-state transport into the nanometer domain, many interesting questions have emerged concerning the solid-state dynamics and quantum transport of carriers in "band-engineered" superlattices and tailored periodic solids.

Foremost among current questions are the age-old, controversial issues concerning the existence of Bloch oscillations and electric-field-induced Stark-ladder energy levels. Recent optical experiments, on excitonic emission from double wells[4] and four-wave mixing from superlattices,[5,6] and optical-absorption studies clearly indicated oscillatory electron dynamics and the manifestation of concomitant Stark-ladder transitions when optical probing is invoked; on the other hand, Bloch oscillations have been elusive in transport experiments, save for several reports of negative differential resistance observations[7-10] ascribed to Bloch oscillatory phase breaking due to the onset of scattering.

No doubt, there is still work to be done in developing the ultimate fundamental resolution of issues concerning the experimental manifestations of Bloch oscillations and the apparent differences observed in transport versus optical-absorption experiments. Resolution of these and other profound issues of quantum transport and optical absorption in the solid state require a fundamental, first-principles description of Bloch-electron dynamics in the presence of homogeneous electric fields of arbitrary strength. Therefore, the purpose of this paper is to extend the zero-order theory of Bloch-electron dynamics in homogeneous electric fields to include implicitly the effects of real band structure in a multiband analysis; as such, the theory derives the dependence of the Zener tunneling time on real band-structure parameters and quantum-mechanical initial conditions.

In this paper, a multiband theory of Bloch-electron dynamics in homogeneous electric fields of arbitrary strength is presented. In this formalism, the electric field is described through the use of the vector potential; in this regard, this work is a major extension of the methodology previously developed by one of the authors (G.J.I.) and co-workers[1-3] to describe solid-state dynamics and quantum transport for Bloch electrons in an applied homogeneous electric field of arbitrary strength and time dependence, including weak scattering from randomly distributed impurities and phonons,[1] and a spatially localized, inhomogeneous electric field.[3] The present paper extends the transition rate theory well beyond the short-time, time-dependent perturbation theory treatment of Krieger and Iafrate[1] to a long-time, multiband analysis. The multiband coupling is treated in the Wigner-Weisskopf (WW) (Ref. 11) approximation, a classic approach for describing the time decay from an occupied quasistationary state; the WW approximation allows

0163-1829/94/50(11)/7553(14)/$06.00

Semicond. Sci. Technol. 9 (1994) 815–819. Printed in the UK

Multiband theory of Bloch electron dynamics in electric fields

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Abstract. A novel multiband theory of Bloch electron dynamics in homogeneous electric fields of arbitrary strength and time dependence is presented. In this formalism, the electric field is described through the use of the vector potential. Multiband coupling is treated through the use of the Wigner–Weisskopf approximation, thus allowing for a Bloch electron transition out of the initial band due to the power absorbed by the electric field; also, the approximation ensures conservation of the total transition probability over the complete set of excited bands. The choice of the vector potential gauge leads to a natural set of extended time-dependent basis functions for describing Bloch electron dynamics in a homogeneous electric field; an associated basis set of localized, electric-field-dependent Wannier and related envelope functions are developed and utilized in the analysis to demonstrate the inherent localization manifest in Bloch dynamics in the presence of relatively strong electric fields. From the theory, a generalized Zener tunnelling time is derived in terms of the applied uniform electric field and the relevant band parameters. The analysis shows an electric-field-enhanced broadening of the excited state probability amplitudes, thus resulting in spatial lattice delocalization and the onset of smearing of discrete, Stark ladder and band-to-band transitions due to the presence of the electric field. In addition, the velocities of a Bloch oscillation will be observed only for the electron that is initially in a Bloch state before Zener tunnelling. Further, the influence of electric fields on resonant tunnelling structure is examined.

1. Introduction

Bloch electron dynamics in a homogeneous electric field has been a subject of great interest dating back to the earliest applications of quantum mechanics to solid state physics [1–3]. Even more recently, as modern fabrication technologies continue to drive the study of solid state transport into the nanometre domain, many new and interesting questions have emerged concerning the solid state dynamics and quantum transport of carriers in 'band-engineered' superlattices and tailored periodic solids.

In this paper, a novel multiband theory of Bloch electron dynamics in homogeneous electric fields of arbitrary strength is presented. In this formalism, the electric field is described through the use of the vector potential; in this regard, this work builds on the methodology previously developed by one of the authors (GJI) and co-workers [1–3] to describe solid state dynamics and quantum transport for Bloch electrons in an applied homogeneous electric field of arbitrary strength and time dependence, including weak scattering from randomly distributed impurities and phonons [1], and a spatially localized, inhomogeneous electric field [3]. In addition, multiband coupling is treated in the Wigner–Weisskopf (W–W) [4] approximation, a classic approach for describing the time decay from an occupied quasistationary state; the W–W approximation allows for the analysis of the long-time, time-dependent tunnelling characteristics of an electron transition out of an initially occupied band due to the power absorbed by the electric field, while preserving conservation of total transition probability over the complete set of excited bands.

The choice of the vector potential gauge leads to a natural set of basis functions for describing Bloch electron dynamics in a homogeneous electric field. A basis set of localized, electric-field-dependent Wannier functions and associated envelope equations are developed to accommodate the inherent localization manifest in Bloch dynamics due to a relatively strong electric field.

Building on previous methodology [3], use is made of the instantaneous eigenstates of the Hamiltonian describing a Bloch electron in an electric field

$$H = \frac{1}{2m}\left(\boldsymbol{P} - \frac{e}{c}A_0(t)\right)^2 + V_c(\boldsymbol{x}) \qquad (1)$$

where $V_c(x)$ is crystal potential. $A_0 = -c\boldsymbol{E}_0 t$ is the vector potential for the time-independent homogeneous electric field, $\boldsymbol{E}_0$, turned on at initial time $t = 0$. The solution

Inst. Phys. Conf. Ser. No 141: Chapter 7
Paper presented at Int. Symp. Compound Semicond., San Diego, 18–22 September 1994

Tight-binding Calculation of Linear Optical Properties of $In_{0.53}Ga_{0.47}As$ Alloys and Heterostructures

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Abstract

We present theoretical calculations of the dielectric function $\varepsilon(\omega)$ of $In_{0.53}Ga_{0.47}As/InP$ superlattices, using the empirical tight-binding (TB) description of electronic states. We demonstrate that the absorption spectra of the constituent bulk materials can be reproduced very well with an appropriate choice of values for optical matrix elements between (TB) basis functions. These parameters then yield the absorption spectra of superlattices. We have computed the imaginary part of the dielectric function, $\varepsilon_2(\omega)$, for ultrathin $(In_{0.53}Ga_{0.47}As)_n/(InP)_n$ superlattices, for $n = 1, 2$, and 3. It is found to be almost identical in all 3 cases. The dominant E_1 and E_2 peaks of $\varepsilon_2(\omega)$ of the superlattices are located in between the corresponding peaks of bulk $In_{0.53}Ga_{0.47}As$ and InP. $\varepsilon_2(\omega)$ is found to be identical for light polarized parallel or perpendicular to growth direction.

I Introduction

$In_xGa_{1-x}As$ alloys and their heterostructures with wider bandgap semiconductors such as InP have emerged as important materials for optoelectronic applications during the past two decades. Examples of such applications include photodetectors, LED's and double-heterostructure lasers for low-loss, low-dispersion optical fiber communication. Many of these applications require a knowledge of the dielectric function $\varepsilon(\omega)$ [1], which is a fundamental material parameter related to the energy band structure and optical matrix elements between valence and conduction band states. In bulk semiconductors $\varepsilon(\omega)$ is adequately modeled by analytic expressions derived using $\mathbf{k} \cdot \mathbf{p}$ theory. Here the dominant contribution to $\varepsilon(\omega)$ comes from interband critical points [2, 3]. The contribution from each critical point may be calculated using parabolic energy bands and a constant momentum matrix element.